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Atomic Structure of Inorganic Nanoparticles: Challenges and Opportunities

Jingyue (Jimmy) Liu

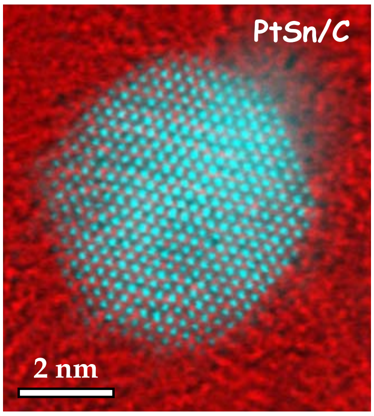
Center for Nanoscience, Department of Physics and Astronomy, Department of Chemistry and Biochemistry, University of Missouri-St. Louis, One University Boulevard, St. Louis, Misoouri 63121, USA. liuj@umsl.edu

Abstract – Understanding the atomic structure of inorganic nanoparticles and other types of nanostructures is a grand challenge in nanoscience and nanotechnology. The recent development of aberration-corrected electron microscopes and associated techniques can provide unprecedented information on the shape, composition and surface atomic arrangement of nanoparticles and nanoclusters. Although many challenges still exist such atomic scale information will help us understand the nature of nanostructures, their formation processes and how to control their synthesis parameters in order to obtain nanostructures with desired properties.

The functional properties (optical, magnetic, electrical, catalytic, etc.) of inorganic nanoparticles are controlled by their size, shape, composition, the arrangement of surface atoms, and the interaction between the nanoparticles and their supports. A comprehensive knowledge of the atomic structure of inorganic nanoparticles is critical to understanding their synthesis-structure-performance relationships and is of practical industrial applications such as the development of nanostructured catalysts with significantly improved selectivity, activity and stability.

Nanoparticles and nanoclusters lack the translational symmetry and long-range order of macro or bulk materials. For small clusters or particles, the specific arrangements of surface atoms determine their physicochemical properties. Structural deviations from their bulk structure become significant when the size of the inorganic nanoparticles decreases to nanometer scale and the shape of nanoparticles becomes an important parameter governing their properties. Detailed information on atomic steps, facets, edges, kinks and surface reconstruction are required if we want to understand the chemical/catalytic properties of nanoparticles and nanoclusters. The dynamic interaction of nanoparticles with their environment (solid, liquid or gas molecules) and their stability under various conditions are fundamental to understanding the performance of nanoparticle systems. Understanding the atomic structure of inorganic nanoparticles or other types of nanostructures is a grand challenge in nanoscience and nanotechnology.

Diffraction techniques, vital to solving structures of inorganic materials, have limited application to characterizing ultra small nanoparticles or nanoclusters since these materials provide only broad diffuse diffraction peaks; to extract reliable and accurate information on the atomic structure, especially surface atomic structure, of nanoparticles or nanoclusters from these diffuse peaks poses significant challenges. On the other hand, the recent advance of aberration-corrected electron microscopes and associated techniques makes it possible to directly image the arrangement of surface atoms of nanoparticles, to analyze their composition, and to determine their electronic structure.



The figure on the right-hand side shows an atomic resolution image of a PtSn alloy nanoparticle formed *in situ* from a Pt_2Sn_2 molecular precursor material. The Pt_2Sn_2 precursor molecules were dispersed onto the Vulcan XC-72 carbon and were then heated *in situ* to form carbon supported PtSn alloy nanocatalysts for direct ethanol fuel cell applications. The RGB image was constructed from a high-angle annular dark-field image (the alloy nanoparticle) and the simultaneously acquired bright-field image (background carbon support) to reveal both the shape of the PtSn alloy nanoparticle and the structure of the carbon support material. The cubo-octahedral alloy nanoparticle shows predominantly {111} surfaces. Such images can provide important information for correlating the shape and structure of nanoparticles with their physicochemical properties.

Atomic level investigations of nanoclusters and nanoparticles and their interactions with supports, as well as their *in situ* synthesis processes and structural evolutions, provide us great opportunities to study the fundamental structure of inorganic nanoparticles and nanoparticle systems [1].

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